Parallel plates and critical exponents for periodic and antiperiodic boundary conditions

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We introduce a renormalized $1PI$ *vertex part scalar field theory setting in momentum space to computing the critical exponents* ν *and* η*, at least at two-loop order, for a layered parallel plate geometry separated by a distance* L*, with periodic as well as antiperiodic boundary conditions on the plates. We utilize massive as well as massless fields in order to extract the exponents in independent ultraviolet and infrared scaling analysis, respectively, which are required in a complete description of the scaling regions for finite size systems. Avoiding the crossover regimes, the three regions of finite size scaling present for each of these boundary conditions are shown to be indistinguishable in the results of the exponents in periodic and antiperiodic conditions, which coincide with those from the (bulk) infinite system.*

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Finite-size effects manifest themselves generically whenever particles or fields are confined within a given volume whose limiting surfaces are separated by a certain distance L. Their size and shape can affect key properties of the system in comparison with those obtained from the $L \to \infty$ limit ("bulk system"). Perhaps the most investigated aspects are related to critical properties of finite systems [1,2], where field-theoretic methods can be employed in the vicinity of the phase transitions taking place in the system under consideration. Experimentally, the simplest realization of such critical behavior and the role played by the finite size corrections show up in parallel plate geometries, for instance, in coexistence curves of critical films of certain fluids [18] as well as superfluid transition features (e.g., specific heat amplitudes) in confined ^{4}He [4,5]. From the theoretical viewpoint, field theory studies have been put forth to explain these effects not only for ^{4}He [6], but also in thin slabs [7,8] formed by wetting phenomena [9]. The Casimir effect has also been investigated in superfluid wetting films [10]. Plus, the recent study of some microscopic properties of finite-lenght cobalt nanowires [11] reveals that the influence of the finiteness is a ubiquitous theme in several properties of physical systems.

Momentum space ϵ-expansion description of critical properties of finite size systems was presented some time ago by Nemirovsky and Freed (NF) [12]. The simplest approach uses a parallel plate geometry, whose plates are of infinite extent along $(d-1)$ spatial directions separated by a distance L. They are subject to geometric restrictions in the form of (periodic, antiperiodic, Dirichlet and Neumann) boundary conditions which are implemented in the bare propagator. The limitation caused by the boundary conditions provides a scaling variable $\frac{L}{\xi_\infty}$, where ξ_∞ is the (bulk) correlation length of the infinite system. For generic boundary conditions, it was conjectured that there could exist three regions induced by the limitation, when: a)$\frac{L}{\xi_\infty} > 1$ where perturbative methods can be applied and the physics is quasi d-dimensional, characterized by bulk critical exponents; b)$\frac{L}{\xi_\infty} = 1$ and the behavior is neither d-dimensional nor $(d-1)$-dimensional; c)$\frac{L}{\xi_\infty} < 1$ where the physics is almost $(d-1)$-dimensional and usual perturbation expansions break down.

In this Letter, we compute the critical exponents η and ν in finite size scaling using the NF method in momentum space, at least up to two-loop order, from a purely analytical perspective when the limiting surfaces separated by a distance L are parallel plates whose order parameter obey either periodic (PBC) or antiperiodic (ABC) boundary conditions on them. We utilize massive fields obeying these boundary conditions on the plates for nonvanishing values of L corresponding to fixed finite values of the bulk correlation length. Region a) can be described satisfactorily in the limit $L \to \infty$ within this massive framework. The remaining regions are treated with massless fields having infinite bulk correlation length. Situation b) is associated to the limit $L \sim \xi_\infty \to \infty$, whereas the c) alternative naturally describes arbitrary finite values of L. The universal results obtained are valid for the three regions determined by the boundedness vari-

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able $\frac{L}{\xi_\infty}$ *with arbitrary nonzero values of* L. *The physics of the systems in the three regions is actually quasi d-dimensional*, for the bulk critical exponents are recovered from the finite size evaluation irrespective of the boundary condition and the value of L. Moreover, we find that *there is no breakdown of the ϵ-expansion into region c)*. The main meaning of our labor, apart from the fact that it represents important progress in the investigation of criticality in parallel plate geometries, is that it illustrates the power of the momentum space approach in the study of finite size systems. The momentum conservation within the region between the plates is responsible for keeping the bulk critical behavior in PBC and ABC.

The layered system can be described by the bare Lagrangian density

$$L = \frac{1}{2}|\bigtriangledown \phi_0|^2 + \frac{1}{2}\mu_0^2\phi_0^2 + \frac{1}{4!}\lambda_0\phi_0^4, \qquad (1)$$

where ϕ_0, μ_0 and g_0 are the bare order parameter, mass (square root of the bare reduced temperature) and coupling constant, respectively [13]. The coordinates are split in the form $x = (\vec{\rho}, z)$ where $\vec{\rho}$ is a $(d-1)$-dimensional vector characterizing the surface of each plate (arbitrarily placed at $z = 0$ and $z = L$) perpendicular to the z direction; the field satisfies $\phi_0(z = 0) = \phi_0(z = L)$ for periodic boundary conditions, whereas $\phi_0(z = 0) = -\phi_0(z = L)$ for antiperiodic boundary conditions. The order parameter can be expanded in Fourier modes as $\phi_0(\vec{\rho}, z) = \Sigma_j \int d^{d-1}k exp(i\vec{k}.\vec{\rho})u_i(z)\phi_{0i}(\vec{k})$, where $\vec{k}$ is the momentum vector associated to the $(d-1)$-dimensional space, $u_j(z)$ are the normalized eigenfunctions of the operator $\frac{d^2}{dz^2}$ whose eigenvalues κ_j defined by $-\frac{d^2u_j(z)}{dz^2} = \kappa_j^2 u_j(z)$ are called the quasi-momentum along the z-direction. In addition, the eigenfunctions obey the relations $\Sigma_j u_j(z)u_j(z') = \delta(z-z')$ and $\int dz u_j(z)u_{j'}(z) = \delta_{jj'}$. Note that $\kappa_j = \sigma(j+\tau)$, where $\sigma = \frac{2\pi}{L}$, $j = 0, \pm1, \pm2, ...$, the label $\tau = 0$ corresponds to PBC and $\tau = \frac{1}{2}$ to ABC. The Feynman rules are modified as follows: beyond the standard tensorial couplings of the infinite theory corresponding to a N component order parameter, each momentum line (propagator) must be multiplied by $\delta_{j_1 j_2}$ and the vertices are multipled by the tensor $S_{j_1j_2j_3j_4} = \int dz u_{j_1}(z)u_{j_2}(z)u_{j_3}(z)u_{j_4}(z)$. The eigenfunctions actually depend on τ and can be written as $u_j^{(\tau)}(z) = L^{-\frac{1}{2}} exp(i\kappa_j z)$ which implies $S_{j_1j_2j_3j_4} = L^{-1}\delta_{j_1+j_2+j_3+j_4,0}$. For each momentum integral in the infinite system perform the substitution $\int d^dk \rightarrow \Sigma_{-\infty}^{\infty}\sigma \int d^{d-1}k$. The bare massive free propagator ($\mu_0^2 \neq 0$) for either boundary condition is given by the expression $G_0^{(\tau)} = \frac{1}{k^2+\sigma^2(j+\tau)^2+\mu_0^2}$.

Considering an arbitrary $1PI$ divergent bare vertex part including composite operators $\Gamma^{(N,M)}$ ($(N,M) \neq (0,2)$), the statement of multiplicative renormalizability amounts to finding renormalization functions Z_ϕ, Z_{ϕ^2} such that the vertex parts defined by $\Gamma_R^{(N,M)} = Z_\phi^{\frac{N}{2}} Z_{\phi^2}^M \Gamma^{(N,M)}$ are automatically finite.

In the massive framework, the primitive divergent vertex parts of this $\lambda\phi^4$ field theory are chosen to be renormalized in the standard way [13], with the choice that the renormalized mass μ be independent of the boundary condition. Setting the symmetry point at zero external momenta for all renormalized quantities, μ is defined by the relation $\Gamma_R^{(2)}(k = 0, j = 0, g, \mu) = \mu^2 + \sigma^2\tau^2$ [6], where g is the renormalized coupling constant determined by $\Gamma_R^{(4)}(k = 0, j = 0, g, \mu) = g$. In addition, $\Gamma_R^{(2,1)}(k = 0, j = 0, g, \mu) = 1$. These conditions are sufficient to formulate all vertex parts which can be renormalized multiplicatively. Recalling that the infrared divergences are absent in the massive theory, we analyze the theory at the ultraviolet region where the momentum of the internal propagators in arbitrary loop graphs are very large, i.e., at the scaling region $\frac{p}{\mu} \rightarrow \infty$ [14].

The one-loop integral contributing to the four-point function is then given by:

$$I_2^{(\tau)}(k', i; \sigma, \mu) = \sigma\Sigma_{j=-\infty}^{\infty} \int d^{d-1}q \frac{1}{[(q)^2+(\sigma)^2(j+\tau)^2+\mu^2]} \times \frac{1}{[(q+k')^2+(\sigma)^2(j+i+\tau)^2+\mu^2]}. \qquad (2)$$

Performing the transformation $p' = \frac{p}{\mu}$ in all momenta present in the diagram and defining $r = \frac{\sigma}{\mu} \propto (\frac{\xi}{L})$, we use Feynman parameters to resolving the integral over q. Then, the remaining summation turns out to be proportional to the generalized thermal function [15]

$$D_\alpha(a, b) = \Sigma_{n=-\infty}^{\infty}[(n+a)^2 + b^2]^{-\alpha} = \frac{\sqrt{\pi}}{\Gamma(\alpha)}\left[\frac{\Gamma(\alpha-\frac{1}{2})}{b^{2\alpha-1}} + f_\alpha(a, b)\right], \qquad (3)$$

with $f_\alpha(a, b) = 4\sum_{m=1}^{\infty} cos(2\pi ma)(\frac{\pi m}{b})^{\alpha-\frac{1}{2}} K_{\alpha-\frac{1}{2}}(2\pi mb)$, and $K_\nu(x)$ is the modified Bessel function of the second kind. Whenever we perform a loop integral, the area of the unit sphere S_d naturally takes place and this angular factor can be neutralized in a redefinition of the coupling constant. We adopt this procedure henceforward in all loop integrals and suppress this overall factor. We then find

$$I_2^{(\tau)}(k', i; \sigma, \mu) = \frac{\mu^{-\epsilon}}{\epsilon}\Big((1-\frac{\epsilon}{2})\int_0^1 dx[x(1-x)(k'^2 + r^2i^2) + 1]^{-\frac{\epsilon}{2}} + \frac{\epsilon}{2}F_{\frac{1+\epsilon}{2}}^{(\tau)}(k', i; r)\Big), \qquad (4)$$

where $F_\alpha^{(\tau)}(k', i; r) = \int_0^1 dx f_\alpha\Big(\tau + xi, h(k', i, r)\Big)$ and $h(k', i, r) = r^{-1}\sqrt{x(1-x)(k'^2 + r^2i^2) + 1}$. At the symmetry point $k' = i = 0$, without loss of generality we can choose $\mu^2 = 1$, such that $r = \sigma$. We find $I_2^{(\tau)}(0, 0; \sigma, 1) = \frac{1}{\epsilon}\big((1-\frac{\epsilon}{2}) + \frac{\epsilon}{2}f_{\frac{1}{2}}(\tau, \sigma^{-1})\big)$. The simplest trend to proceed hereafter is to compute the remaining massive diagrams at these values of parameters. The limit $r \rightarrow 0$ neatly represents the region a)

($L \to \infty$ with ξ fixed), where both $F^{(\tau)}_{\frac{1+\epsilon}{2}}(k', i; \sigma = 0)$ and $f^{(\tau)}_{\frac{1+\epsilon}{2}}(k', i; \sigma = 0)$ tend to zero.

The two-loop graph of the four-point function $I_4^{(\tau)}(0, 0; \sigma, 1)$ in terms of the integral $I_2(\tau)(0, 0, \sigma, 1)$ reads

$$I_4^{(\tau)}(0, 0; \sigma, 1) = \sigma \Sigma_{j=-\infty}^{\infty} \int d^{d-1}q \frac{I_2^{(\tau)}(q, j; \sigma, 1)}{[(q)^2 + (\sigma)^2(j+\tau)^2 + 1]^2}. \quad (5)$$

It can be carried out similarly and results in the expression $I_4^{(\tau)}(0, 0; \sigma, 1) = \frac{1}{2\epsilon^2}\big((1 - \frac{\epsilon}{2}) + \epsilon f_{\frac{1}{2}}(\tau, \sigma^{-1})\big)$.

Next, we need the two-point function diagrams. The calculation of the derivative of the two-loop "sunset" diagram $I_3^{(\tau)}$ and the three-loop diagram $I_5^{(\tau)}$ with respect to k'^2 denoted by $I_3'^{(\tau)}$ and $I_5'^{(\tau)}$ (at null k'), respectively, are required. In terms of the building block $I_2^{(\tau)}(k', i; \sigma, 1)$ we can write

$$I_3^{(\tau)}(k, i; \sigma, 1) = \sigma \Sigma_{j=-\infty}^{\infty} \int d^{d-1}q \frac{I_2^{(\tau)}(q + k, j + i; \sigma, 1)}{[(q)^2 + \sigma^2(j+\tau)^2 + 1]}, \quad (6a)$$

$$I_5^{(\tau)}(k, i; \sigma, 1) = \sigma \Sigma_{j=-\infty}^{\infty} \int d^{d-1}q \frac{[I_2^{(\tau)}(q + k, j + i; \sigma, 1)]^2}{[(q)^2 + (\sigma)^2(j+\tau)^2 + 1]}. \quad (6b)$$

Now $F^{(\tau)}_{\alpha,\beta}(k, i; \sigma) \equiv \frac{1}{S_d}\sigma \Sigma_{j=-\infty}^{\infty} \int d^{d-1}q \frac{F^{(\tau)}_{\alpha}(q+k, j+i; \sigma, 1)}{[(q)^2+(\sigma)^2(j+\tau)^2+1]^{\beta}}$, such that $F'^{(\tau)}_{\alpha}(\sigma) = \frac{\partial F^{(\tau)}_{\alpha,1}(k,i;\sigma)}{\partial k^2}\big|_{(k,i)=0}$. The parametric integrals

$$I^{(\tau)}(\sigma) = -2\int dxdyy \quad \times$$
$$ln\big[y(1-y)\tau^2\sigma^2 + y + \tfrac{1-y}{x(1-x)}\big] - \tfrac{1}{2}, \quad (7a)$$
$$G^{(\tau)}(\sigma) = 2\int dxdyy \quad \times$$
$$f_{\frac{1}{2}}\Big(y\tau, \sqrt{y(1-y)\tau^2 + \sigma^{-2}y + \tfrac{\sigma^{-2}(1-y)}{x(1-x)}}\Big), \quad (7b)$$

will also be requested. Evaluation of the integrals yield the values $I_3'^{(\tau)}(0, 0; \sigma, 1) = -\frac{1}{8\epsilon}\big(1 - \frac{\epsilon}{4} + \epsilon W^{(\tau)}(\sigma)\big)$ and $I_5'^{(\tau)}(0, 0; \sigma, 1) = -\frac{1}{6\epsilon^2}\big(1 - \frac{\epsilon}{4} + \frac{3\epsilon}{2}W^{(\tau)}(\sigma)\big)$, where $W^{(\tau)}(\sigma) = I^{(\tau)}(\sigma) + G^{(\tau)}(\sigma) - 4F_0'^{(\tau)}(\sigma)$.

From the eigenvalue condition $\beta(u_\infty) = 0$, we learn that the repulsive ultraviolet fixed point is given by

$$u_\infty = \big(\frac{6}{N+8}\big)\epsilon\big[1 + \epsilon\big(\frac{9N+42}{(N+8)^2} + \frac{1}{2}(1 - f_{\frac{1}{2}}(\tau, \sigma^{-1}))\big)\big]. \quad (8)$$

At three-loop order, the function responsible for the anomalous dimension of the field

$$\gamma_\phi^{(\tau)}(\sigma, u) = \frac{(N+2)}{72}u^2\big[1 - \frac{\epsilon}{4} + \epsilon W^{(\tau)}(\sigma) - \frac{N+8}{6}(1 + W^{(\tau)}(\sigma) - f_{\frac{1}{2}}(\tau, \sigma^{-1}))u\big], \quad (9)$$

is actually dependent upon the boundary condition, but turns out to become insensitive to them at the fixed point. Indeed, $\gamma_\phi^{(\tau)}(\sigma, u_\infty) = \eta = \frac{(N+2)}{2(N+8)^2}\epsilon^2\{1 + \epsilon\big[\frac{6(3N+14)}{(N+8)^2} - \frac{1}{4}\big]\}$. The same happens to the composite field Wilson function, given explicitly by the expression

$$\gamma_{\phi^2}^{(\tau)}(\sigma, u) = \big(\frac{N+2}{6}\big)\big[1 - \frac{\epsilon}{2}(1 - f_{\frac{1}{2}}(\tau, \sigma^{-1}))\big]u - \frac{(N+2)}{12}u^2, \quad (10)$$

which at the fixed point results in the expression $\gamma_{\phi^2}^{(\tau)}(\sigma, u_\infty) = \frac{(N+2)}{(N+8)}\epsilon\big[1 + \epsilon\frac{(6N+18)}{(N+8)^2}\big]$. Using the scaling relation $\nu^{-1} = 2 - \eta - \gamma_{\phi^2}^{(\tau)}(\sigma, u_\infty)$, we find $\nu = \frac{1}{2} + \frac{N+2}{4(N+8)}\epsilon + \frac{(N+2)(N^2+23N+60)}{8(N+8)^3}\epsilon^2$.

In the massless approach the bulk correlation length is infinite, so infinite values of L will lead to the situation $\frac{L}{\xi_\infty} \to 1$, whereas finite values of L represents the region $\frac{L}{\xi_\infty} \to 0$. The scaling region now occurs in the infrared regime. The bare free critical propagator is now $G_0^{(\tau)} = \frac{1}{k^2+\sigma^2(j+\tau)^2}$. The renormalized vertices are defined as before, but the symmetry point of the renormalized theory must be chosen at nonvanishing external momenta along $(d-1)$ spatial directions, say κ [13], and external quasi-momentum $j = 0$. The two-point function is renormalized according to $\Gamma_R^{(2)}(k = 0, j = 0, g, 0) = \sigma^2\tau^2$, where g is the renormalized coupling determined by $\Gamma_R^{(4)}(k_i, j = 0, g, \mu)|_{SP} = g$ and $\Gamma_R^{(2,1)}(\kappa, j = 0, g, 0)|_{\bar{SP}} = 1$. We fix the scale of the external momenta at the symmetry point as $\kappa^2 = 1$. It is important to emphasize that the same angular factor already discussed in the massive theory appears every time we perform a loop integral and shall be absorbed from now on in a redefinition of the coupling constant just as before.

We are left with the computation of the massless integrals Eqs. (2), (5), (6) for nonvanishing external momenta, which are even simpler than their massive counterparts. When the value of the diagrams are substituted back in the β-function, the condition $\beta(u^*) = 0$ yields the trivial solution $u^* = 0$ as well as the attractive infrared nontrivial fixed point, namely

$$u^* = \big(\frac{6}{N+8}\big)\epsilon\big[1 + \epsilon\big(\frac{9N+42}{(N+8)^2} - \frac{1}{2}(1 + \tilde{F}_0^{(\tau)}(k^2 = \kappa^2 = 1, i = 0))\big)\big], \quad (11)$$

where

$$\tilde{F}_\beta^{(\tau)}(k, i) = \int_0^1 dx f_\beta\Big(\tau + ix, \tilde{h}(k, i, \sigma)\Big), \quad (12)$$

and $\tilde{h}(k,i,\sigma) = \sqrt{x(1-x)(i^2+\frac{k^2}{\sigma^2})}$. The other definitions are exactly the same as in the massive approach where a quantity, say F is replaced by its massless counterpart $\tilde{F}$. Finally, define the object $\bar{F}_{\beta}^{(\tau)}(k) = \sigma^{-2\beta}\int_0^1 dyy(1-y)^{\frac{\beta}{2}} f_{\frac{1}{2}+\beta}(y\tau, \tilde{h}(k, i=0,\sigma))$. At $k^2 = 1, i=0$, the combination $\tilde{W}^{(\tau)} = \frac{1}{2}ln[1+\sigma^2\tau^2]+2\tilde{F}'^{(\tau)}_0 - \bar{F}_0^{(\tau)}$ is worthwhile. In fact, the Wilson functions read:

$$\gamma_{\phi}^{(\tau)}(u) = \frac{(N+2)}{72}u^2\Big[1+\frac{5\epsilon}{4} - 2\epsilon\tilde{W}^{(\tau)} - \frac{(N+8)}{12}(1 - 4\tilde{W}^{(\tau)} - 2\tilde{F}_0^{(\tau)}(k^2=\kappa^2=1, i=0))u\Big], \quad (13a)$$

$$\gamma_{\phi^2}^{(\tau)}(u) = \frac{(N+2)}{6}u(1+\frac{\epsilon}{2} + \frac{1}{2}\epsilon\tilde{F}_0^{(\tau)}(k^2=\kappa^2=1, i=0) - \frac{u^2}{2}). \quad (13b)$$

When these functions are computed at the fixed point, the same critical exponents ν and η arise independent of the boundary conditions. Therefore, we proved the equivalence of the infrared and ultraviolet scaling regimes for finite systems using PBC and ABC, i.e., the results are valid independently of the limitation parameter $\frac{L}{\xi_\infty}$, provided the crossover regions where the ϵ-expansion breaks down is avoided.

In conclusion, our findings represent cutting-edge results for this field-theoretic momentum space computation of observables using finite size arguments at least up to two-loop level, formulated with normalization conditions for the renormalized two-point vertex parts which depend on the boundary conditions. They shall pave the road to compute amplitudes in massive as well as massless framework at higher orders in renormalized perturbation theory [16]. The detailed discussion of the picture presented here, including the minimal subtraction procedure in the massless formalism will be published elsewhere.

It would be interesting to carry out the same analysis at least at two-loop order in more complicated situations involving Dirichlet and Neumann boundary conditions, since they are more appealing from the phenomenological viewpoint. They characterize free surfaces [17], which disturb further the system due to the breaking of translational invariance along the finite directions. We expect that boundedness independence can also be achieved in Dirichlet and Neumann boundary conditions, provided the dimensional crossover regimes (already verified experimentally in thin films of a critical mixture of 2,6-lutidine+water [18]) is avoided likewise. New features appear due to nonconservation of the quasi-momentum for those cases which deserve a careful treatment.

Finally, it would be desirable to adapt the description worked out herein to the case of competing systems of the Lifshitz type [19–21]. It remains to be seen if the competing axes with arbitrary momentum powers permit exact results when the finite size direction points along any of them.

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